

Rec'd PCT 21 JAN 2005

INTERNATIONAL SEARCH REPORT

International application No.

PCT/IL02/00614

A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) : G01N 31/00, 33/48; G06F 19/00

US CL : 702/19,22,27

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 702/19,22,27

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
STN on line

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X --- Y	FEJZO et al. The SHAPES strategy: an NMR-based approach for lead generation in drug discovery. Chemistry & Biology, October 1999, Vol. 6, No. 10, pages 755-769. See abstract.	1-7,36,41- 43,57,102,103 ----- 14,15,24-35,44-46
X --- Y	SANNES-LOWERY et al. High-performance mass spectrometry as a drug discovery tool: a high-throughput screening assay to identify RNA-binding ligands. Proceedings of SPIE-The International Society for Optical Engineering (2001), Vol. 4264, pages 27-36. See abstract.	1-7,36,41- 43,57,102,103 ----- 14,15,24-35,44-46
Y	DARVAS, F. et al. A Photoactivatable Library Approach for Target Identification and Validation. Publisher: American Chemical Society, Washington, D.C., April 2002, see abstract #MEDI-245.	1-7,14,15,24-36,41- 46,57,102,103
A	WO 98/16835 A2 (TERRAPIN TECHNOLOGIES, INC.) 23 April 1998 (23.04.1998), entire document.	36,41-46,57,102,103

☐ Further documents are listed in the continuation of Box C.

☐ See patent family annex.

Special categories of cited documents:

- *"A" document defining the general state of the art which is not considered to be of particular relevance
- *"E" earlier application or patent published on or after the international filing date
- *"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- *"O" document referring to an oral disclosure, use, exhibition or other means
- *"P" document published prior to the international filing date but later than the priority date claimed

- *"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
- *"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
- *"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
- *"&" document member of the same patent family

Date of the actual completion of the international search

08 July 2003 (08.07.2003)

Date of mailing of the international search report

19 AUG 2003

Name and mailing address of the ISA/US

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Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claim Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☐ Claim Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:
3. ☐ Claim Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:
Please See Continuation Sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.: 1-7, 14, 15, 24-36, 41-46, 57, 102, 103

Remark on Protest ☐ The additional search fees were accompanied by the applicant's protest.
☐ No protest accompanied the payment of additional search fees.

BOX II. OBSERVATIONS WHERE UNITY OF INVENTION IS LACKING

Group I, claims 1-57, 102, 103, drawn to methods of obtaining information about active area of a target molecule.

Group II, claims 58-60, drawn to method of identifying existence of plurality of chemical-spatial configurations in a target molecule.

Group III, claims 61-68, drawn to method of reconstructing spatial shape of chemical binding configuration.

Group IV, claims 69-75, drawn to method for selecting a scaffold.

Group V, claims 76-82, drawn to method for selecting a gauge molecule.

Group VII, claims 85-89, drawn to method for reducing screening library.

Group VIII, claims 90-101, drawn to method for designing a screening library.

Group IX, claims 104, 105, drawn to lead set.

Group X, claims 106, drawn to a drug lead.

Group XI, claims 107-126, drawn to first screening library comprising at least 10,000 molecules derived from scaffold molecules.

Group XII, claims 127-134, drawn to second screening library comprising rigid molecules.

Group XIII, claims 135-146, drawn to third screening library comprising gauge molecules.

Group XIV, claims 147-151, drawn to method of obtaining information.

Group XV, claims 152-154, drawn to method of constructing a lead.

In addition, Group I of this application contains claims directed to more than one species of the generic invention. The species identified below are deemed to lack Unity of Invention because they are not so linked as to form a single inventive concept under PCT Rule 13.1. In order for more than one species to be examined, the appropriate additional search fees must be paid. The species are as follows:

- A. For claims 7-13, 5 species of "identifying", such as identifying configuration that matches configuration of a bound gauge, does not match configuration of a bound gauge, identifying by statistical analysis, by clustering, etc.
- B. For claims 14-16, 2 species of "reconstructing", such as based on assay results, or based on configurations.
- C. For claims 18, 19 - 2 species of reconstruction steps, such as based on scoring maps, or on maps clustering.
- D. For claims 36-39 - 4 species of assay types, such as functional, binding, cellular, flow-through.
- E. For claims 50-52 - 3 species of utilizing lead in map analysis: selecting a lead, rejecting a lead, constructing a lead. The inventions listed as Groups I-VIII, Xiv, Xv do not related to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Each of the Groups claim a distinct and separate method. The methods do not share a special technical feature because each method contains specific and unique method steps which are not shared by each of the other methods and each method has a unique and distinct outcome. Thus, group I-VIII, XIV, XV do not share a corresponding special technical feature.

The inventions listed as Groups IX-XII do not relate to a single general inventive concept under PCT rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features: the libraries are produced by different methods, and there is no common core structure identified for said libraries of compounds.